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     FILE 'HCAPLUS' ENTERED AT 17:10:51 ON 19 APR 2007
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                E US6420359/PN 25
L2
              1 S E3
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L3
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L8
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     FILE 'HCAPLUS' ENTERED AT 17:31:20 ON 19 APR 2007
                E RITONAVIR+ALL/CT
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497529 S (RITONAVIR OR "CHEMICAL COMPOUNDS") OR "ORGANIC COMPOUNDS" OR

E RITONAVIR+ALL/CT

E RITONAVIR+ALL/CT

2647 S RITONAVIR

11 S L1-L10

9 S L15 AND L13

4 S L7

Roy P. Issac

L12

L13

L14

L15

L16

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2004:531365 HCAPLUS DOCUMENT NUMBER: 141:65063 Use of a combination containing a non-nucleoside TITLE: reverse transcriptase inhibitor (NNRTI) with an inhibitor of cytochrome p450 for the treatment of HIV-1 infection Cordingley, Michael Graham INVENTOR(S): PATENT ASSIGNEE(S): Boehringer Ingelheim International GmbH, Germany SOURCE: PCT Int. Appl., 23 pp. CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION: WO 2004054586 21 PATENT NO. KIND DATE APPLICATION NO. A1 20040701 WO 2003-EP14224 20031215 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, A1 20040701 CA 2003-2510143 20031215 A1 20040709 AU 2003-296647 20031215 A1 20040805 US 2003-736301 20031215 A1 20050921 EP 2003-813119 20031215 CA 2510143 AU 2003296647 US 2004152625 20031215 <--EP 1575595 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

 BR 2003017095
 A
 20051025
 BR 2003-17095
 20031215

 CN 1726041
 A
 20060125
 CN 2003-80106301
 20031215

 JF 2006511538
 T
 20060406
 JP 2004-560402
 20031215

 NC 2005003455
 A
 20050810
 NO 2005-3455
 20050715

 US 2002-433690P P 20021216 WO 2003-EP14224 W 20031215 PRIORITY APPLN. INFO.: AB An improved method for using a NNRTI in the treatment of HIV-1 infection comprises administering to a human in need of treatment for HIV-1 infection a therapeutically effective amount of the NNRTI, or a pharmaceutically acceptable salt thereof, and an amount of an inhibitor of cytochrome P 450 that is sufficient to elevate, enhance, or extend plasma concns. of said NNRTI. 380378-81-4 IT RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (non-nucleoside reverse transcriptase inhibitor combination with

cytochrome P 450 inhibitor for treatment of HIV-1 infection)

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]- (9CI) (CA INDEX NAME)

Roy P. Issac

RN CN 380378-81-4 HCAPLUS

IT 380378-81-4D, mixts. with grapefruit juice 710282-29-4 710282-30-7 710282-31-8 710282-32-9 710282-33-0 710282-34-1 710282-35-2 710282-36-3 710282-37-4 710282-38-5 710282-39-6 710282-40-9 710282-41-0 71.0282-42-1 710282-43-2 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (non-nucleoside reverse transcriptase inhibitor combination with cytochrome P 450 inhibitor for treatment of HIV-1 infection) RN 380378-81-4 HCAPLUS CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]- (9CI) (CA INDEX NAME)

RN 710282-29-4 HCAPLUS
CN 2,5,6,10,13-Pentaazatetradecanedioic acid, 3,12-bis(1,1-dimethylethyl)-8hydroxy-4,11-dioxo-9-(phenylmethyl)-6-[[4-(2-pyridinyl)phenyl]methyl]-,
dimethyl ester, (3S,8S,9S,12S)-, mixt. with 11-ethyl-5,11-dihydro-5-methyl8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-6H-dipyrido[3,2-b:2',3'e][1,4]diazepin-6-one (9CI) (CA INDEX NAME)

CM 1

CRN 380378-81-4 CMF C25 H23 N5 O3

CM 2

CEN 198904-31-3 CMF C38 H52 N6 O7

Absolute stereochemistry. Rotation (-).

RN 710282-30-7 HCAPLUS

CN Erythromycin, 6-O-methyl-, mixt. with 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one (9CI) (CA INDEX NAME)

CM 1

CRN 380378-81-4 CMF C25 H23 N5 O3

CM 2

CEN 81103-11-9 CMF C38 H69 N O13

Absolute stereochemistry.

RN 710282-31-8 HCAPLUS

CN Cyclosporin, mixt. with 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one (9CI) (CA INDEX NAME)

CM 1

CRN 380378-81-4 CMF C25 H23 N5 O3

CM 2

CRN 79217-60-0 CMF Unspecified

CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 710282-32-9 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-, mixt. with

(2S,3S)-3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-1,5-benzothiazepin-4(5H)-one (9CI) (CA INDEX NAME)

CIM 1

CM 2

CRN 42399-41-7 CMF C22 H26 N2 O4 S

Absolute stereochemistry. Rotation (+).

RN 710282-33-0 HCAPLUS CN Erythromycin, mixt.

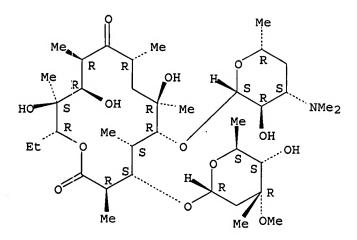
Erythromycin, mixt. with 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one (9CI) (CA INDEX NAME)

CM 1

CM 2

CRN 114-07-8 CMF C37 H67 N O13

Absolute stereochemistry. Rotation (-).



RN 710282-34-1 HCAPLUS CN 6H-Dipyrido[3,2-b:2'

 $6H-Dipyrido[3,2-b:2',3'-e] [1,4] diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-, mixt. with \\ 4-[4-[4-[4-[4-[4-[2-(2,4-dichlorophenyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]phenyl]-2,4-dihydro-2-(1-methylpropyl)-3H-1,2,4-triazol-3-one (9CI) (CA INDEX NAME)$

CM 1

C:M 2

CRN 84625-61-6 CMF C35 H38 Cl2 N8 O4

PAGE 1-A

PAGE 2-A

RN 710282-35-2 HCAPLUS

D-erythro-Pentonamide, 2,3,5-trideoxy-N-[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]-5-[(2S)-2-[[(1,1-dimethylethyl)amino]carbonyl]-4-(3-pyridinylmethyl)-1-piperazinyl]-2-(phenylmethyl)-, mixt. with 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one (9CI) (CA INDEX NAME)

CM 1

CN

CRN 380378-81-4 CMF C25 H23 N5 O3

CM 2

CRN 150378-17-9 CMF C36 H47 N5 O4

Absolute stereochemistry.

RN 710282-36-3 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-, mixt. with rel-1-acetyl-4-[4-[(2R,4S)-2-(2,4-dichlorophenyl)-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]piperazine (9CI) (CA INDEX NAME)

CM 1

CRN 380378-81-4 CMF C25 H23 N5 O3

CM 2

CRN 65277-42-1 CMF C26 H28 Cl2 N4 O4

Relative stereochemistry.

RN 710282-37-4 HCAPLUS

CN Acetic acid, methoxy-, (1S,2S)-2-[2-[[3-(1H-benzimidazol-2-yl)propyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, mixt. with 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one (9CI) (CA INDEX NAME)

CM 1

CRN 380378-81-4 CMF C25 H23 N5 O3

CM 2

CRN 116644-53-2 CMF C29 H38 F N3 O3

Absolute stereochemistry.

RN 710282-38-5 HCAPLUS

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-, mixt. with 2-[3-[4-(3-chlorophenyl)-1-piperazinyl]propyl]-5-ethyl-2,4-dihydro-4-(2-phenoxyethyl)-3H-1,2,4-triazol-3-one (9CI) (CA INDEX NAME)

C:M 1

CN

CRN 380378-81-4 CMF C25 H23 N5 O3

CM 2

CRN 83366-66-9 CMF C25 H32 Cl N5 O2

RN 710282-39-6 HCAPLUS

CN 3-Isoquinolinecarboxamide, N-(1,1-dimethylethyl)decahydro-2-[(2R,3R)-2-hydroxy-3-[(3-hydroxy-2-methylbenzoyl)amino]-4-(phenylthio)butyl]-, (3S,4aS,8aS)-, mixt. with 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one (9CI)

(CA INDEX NAME)

CM 1

CRN 380378-81-4 CMF C25 H23 N5 O3

CM 2

CRN 159989-64-7 CMF C32 H45 N3 O4 S

Absolute stereochemistry.

RN 71.0282-40-9 HCAPLUS

CN 2,4,7,12-Tetraazatridecan-13-oic acid, 10-hydroxy-2-methyl-5-(1-methylethyl)-1-[2-(1-methylethyl)-4-thiazolyl]-3,6-dioxo-8,11-bis(phenylmethyl)-, 5-thiazolylmethyl ester, (5S,8S,10S,11S)-,mixt. with 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one (9CI) (CA INDEX NAME)

CM 1

CM 2

CRN 155213-67-5 CMF C37 H48 N6 O5 S2

Absolute stereochemistry.

RN 710282-41-0 HCAPLUS

CN Vitamin E, mixt. with 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one (9CI) (CA INDEX NAME)

CM 1

CM 2

CRN 1406-18-4 CMF Unspecified

CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 710282-42-1 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-, mixt. with 4-[[(2E)-3,7-dimethyl-2,6-octadienyl]oxy]-7H-furo[3,2-g][1]benzopyran-7-one (9CI) (CA INDEX NAME)

CM 1

CIM 2

CRN 7380-40-7 CMF C21 H22 O4

Double bond geometry as shown.

RN 710282-43-2 HCAPLUS
CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]-, mixt. with

4-[[(2E)-6,7-dihydroxy-3,7-dimethyl-2-octenyl]oxy]-7H-furo[3,2-

g][1]benzopyran-7-one (9CI) (CA INDEX NAME)

CM 1.

CRN 380378-81-4 CMF C25 H23 N5 O3

CM 2

CRN 145414-76-2 CMF C21 H24 O6

Double bond geometry as shown.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:451667 HCAPLUS

DOCUMENT NUMBER: 141:23559

TITLE: Preparation of 5,11-dihydro-8-(2-hydroxyethyl)-6H-

dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one derivatives

as non-nucleoside reverse transcriptase inhibitors

Yoakim, Christiane; Malenfant, Eric; Thavonekham,

Bounkham; Ogilvie, William; Deziel, Robert

PATENT ASSIGNEE(S): Boehringer Ingelheim (Canada) Ltd., Can.

SOURCE: U.S. Pat. Appl. Publ., 27 pp.

CODEN: USXXCO DOCUMENT TYPE: Patent

LANGUAGE: Patent English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

INVENTOR(S):

PATENT NO	o. 		API	LICATION NO.	DATE
US 200410	06791		0603 US	2003-662856	20030915
US 710551	10	B2 2006	0912		
			1007 CA	2003-2495721	20030915
					20030915
					BZ, CA, CH, CN,
					FI, GB, GD, GE,
					KR, KZ, LC, LK,
			•		MZ, NI, NO, NZ,
					SL, SY, TJ, TM,
			• •	C, VN, YU, ZA,	
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					SE, SI, SK, TR,
					NE, SN, TD, TG
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				2003-816107	20030915
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				TR, BG, CZ,	
JP 200651	15312	T 2006	0525 JP	2004-569819	20030915
AT 331716	6	T 2006	0715 AT	2003-816107	20030915
PRIORITY APPL	N. INFO.:		US	2002-411785P	P 20020919
				2003-CA1409	
OTHER SOURCE (S	S):	MARPAT 141:			

Roy P. Issac

AB The title compds. represented by formula (I) [wherein R1 = H, halogen, C1-4 alkyl, C1-4 alkoxy, haloalkyl; R2, R3 = H, C1-4 alkyl; R4 = C1-4 alkyl, C1-4 alkyl-C3-7 cycloalkyl, C3-7 cycloalkyl; Q = a fused phenyl-5 or 6-membered saturated heterocycle having one to two heteroatoms selected from O and N, said Q being optionally substituted with hydroxy, or C1-4 alkyl which in turn maybe optionally substituted with pyridinyl-N-oxide or CO2R (wherein R = H, C1-4 alkyl)] or salts thereof are prepared These compds. have inhibitory activity against wild type HIV and single and double mutants strains of HIV. Thus, Mitsunobu reaction of 2,3-Dihydro-1H-isoindole with 5,11-Dihydro-11-ethyl-8-(2-hydroxyethyl)-5-methyl-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one using DEAD and Ph3P in THF at room temperature for 16 h gave I (R1 = R2 = H, R3 = Me, R4 = Et, Q = 2,3-dihydro-1-oxo-1H-isoindol-4-yl) which showed IC50 of <10 μM against RNA-dependent DNA polymerase of HIV-1 RT.

IT 380378-90-5P, 2-Chloro-N-[2-(ethylamino)-3-pyridinyl]-5-bromo-3-pyridinecarboxamide 380378-91-6P

I

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 5,11-dihydro-8-(2-hydroxyethyl)-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one derivs. as non-nucleoside reverse transcriptase inhibitors and HIV inhibitors)

RN 380378-90-5 HCAPLUS

CN 3-Pyridinecarboxamide, 5-bromo-2-chloro-N-[2-(ethylamino)-3-pyridinyl](9CI) (CA INDEX NAME)

RN 380378-91-6 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl-8-(2-propenyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:267338 HCAPLUS

DOCUMENT NUMBER: 140:303707

TITLE: Preparation of 9H-imidazo[1,2-d]dipyrido[2,3-b:3',2'-

f][1,4]diazepine derivatives as tetracyclic

non-nucleoside reverse transcriptase inhibitors useful

against wild type and double-mutation K103N/Y181C

enzymes

INVENTOR(S): Yoakim, Christiane; O'Meara, Jeffrey; Simoneau, Bruno;

Ogilvie, William W.; Deziel, Robert

PATENT ASSIGNEE(S): Boehringer Ingelheim (Canada) Ltd., Can.

SOURCE: PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.						
WO 2004026875		WO 2003-CA1410						
		BA, BB, BG, BR, BY,						
•		DZ, EC, EE, ES, FI,						
		JP, KE, KG, KP, KR,						
		MK, MN, MW, MX, MZ,						
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		SD, SE, SG, SK, SL,						
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		SL, SZ, TZ, UG, ZM,						
		BE, BG, CH, CY, CZ,						
FI, FR, GB,	GR, HU, IE, IT,	LU, MC, NL, PT, RO,	SE, SI, SK, TR,					
BF, BJ, CF,	CG, CI, CM, GA,	GN, GQ, GW, ML, MR,	NE, SN, TD, TG					
CA 2495744	A1 20040401	CA 2003-2495744	20030915					
AU 2003269628	A1 · 20040408	AU 2003-269628	20030915					
		US 2003-662606						
		EP 2003-750192						
		GB, GR, IT, LI, LU,						
		CY, AL, TR, BG, CZ,						
		JP 2004-536726	•					
PRIORITY APPLN. INFO.:								
PRIORITI APPLIN. INFO.:		US 2002-411745P						
OFFIED COLLEGE (C)		WO 2003-CA1410	W 20030915					
OTHER SOURCE(S):	MARPAT 140:3037	140:303707						

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I are disclosed [wherein: R1 = H, halogen, (C1-4)alkyl, O(C1-4)alkyl, and haloalkyl; R2 = H or Me; R3 = H or (C1-4)alkyl; R4 = H or (C1-4)alkyl; R5 = (C1-4)alkyl, (C1-4)alkyl(C3-7)cycloalkyl, or (C3-7)cycloalkyl; W = benzo-fused 5- or 6-membered heterocycle having one or two N and/or S atoms; W = Ph, 1,1'-biphenyl, 2,3-dihydro-1H-indene, 1,2,3,4-tetrahydronaphthyl, or naphthyl; W being optionally substituted with (C1-4)alkyl, which in turn can be optionally substituted with a carboxy or (C1-4)alkoxycarbonyl; or a salt or ester thereof]. The compds. have inhibitory activity against wild type (WT), single-mutant, and double-mutant strains of HIV, and are particularly potent against WT and double-mutant K103N/Y181C strains of HIV-1 reverse transcriptase (RT). Over 20 compds. I were prepared and tested. For instance, the thione

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intermediate II was prepared in 8 steps from 2-chloro-3-nitropyridine and 5-bromo-2-chloro-3-pyridinecarbonyl chloride. Cyclocondensation of the thioamide function of II with aminoacetaldehyde di-Me acetal to form an imidazole fusion, followed by deprotection, etherification with a carboxy-protected hydroxybiphenylacetic acid derivative, and deprotection, gave title compound III. In assays for inhibition of RT, III had IC50 values of <50 nM for both WT and K103N/Y181C strains of RT. In a cell-based assay against WT HIV-1, III had an EC50 of <10 nM. 380378-90-5P, 2-Chloro-N-[2-(ethylamino)-3-pyridinyl]-5-bromo-3-

pyridinecarboxamide

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of imidazodipyridodiazepine derivs. as non-nucleoside reverse transcriptase inhibitors useful against wild type and double-mutation K103N/Y181C enzymes)

RN 380378-90-5 HCAPLUS

3-Pyridinecarboxamide, 5-bromo-2-chloro-N-[2-(ethylamino)-3-pyridinyl](9CI) (CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:51812 HCAPLUS

DOCUMENT NUMBER: 140:287364

TITLE: Novel nevirapine-like inhibitors with improved

activity against NNRTI-resistant HIV:

8-heteroarylthiomethyldipyridodiazepinone derivatives Yoakim, C.; Bonneau, P. R.; Deziel, R.; Doyon, L.;

Duan, J.; Guse, I.; Landry, S.; Malenfant, E.; Naud,

J.; Ogilvie, W. W.; O'Meara, J. A.; Plante, R.;

Simoneau, B.; Thavonekham, B.; Bos, M.; Cordingley, M.

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CORPORATE SOURCE: Department of Chemistry, Research & Development,

Boehringer Ingelheim (Canada) Ltd, Lava, QC, 2100,

Can.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),

14(3), 739-742

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:287364

GI

AUTHOR (S):

AB A series of 8-heteroarylthiomethyldipyridodiazepinone derivs. were prepared and evaluated for their antiviral profile against wild type virus and the important K103N/Y181C mutant as an indicator for broad activity.

2,6-Dimethylpyridine derivative I was found to have a good pharmacokinetic profile in spite of poor metabolic stability in rat liver microsomes.

380379-06-6
RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of 8-heteroarylthiomethyldipyridodiazepinone derivs. with improved activity against NNRTI-resistant HIV)
380379-06-6 HCAPLUS

RN 380379-06-6 HCAPLUS CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 8-bromo-2-chloro-11-ethyl-5,11-dihydro-4-methyl- (9CI) (CA INDEX NAME)

IT

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:777795 HCAPLUS

DOCUMENT NUMBER: 139:292278

TITLE: Dipyridodiazepinones as reverse transcriptase

inhibitors

INVENTOR(S): O'Meara, Jeffrey; Simoneau, Bruno; Yoakim, Christiane;

Deziel, Robert; Ogilvie, William W.

PATENT ASSIGNEE(S): Boehringer Ingelheim International G.m.b.H., Germany

SOURCE: PCT Int. Appl., 39 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2003080612 A1 20031002 WO 2003-CA418 20030324

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
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                                                                     20030324
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                                             CN 2003-806463
                                                                     20030324
                          Α
                                             JP 2003-578366
     JP 2005521699
                           T
                                 20050721
                                                                     20030324
     IN 2004DN02433
                                             IN 2004-DN2433
                          Α
                                 20070302
                                                                     20040820
     NO 2004004043
                          Α
                                 20040929
                                             NO 2004-4043
                                                                     20040924
PRIORITY APPLN. INFO.:
                                             US 2002-367971P
                                                                     20020327
                                                                  W 20030324
                                             WO 2003-CA418
OTHER SOURCE(S):
                         MARPAT 139:292278
GΙ
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This invention provides the compds. I (R = H, halogen, (C1-4)alkyl, O(C1-4)alkyl, NH(C1-4alkyl) or N(C1-4alkyl)2; R1 = H or Me; R2 = H or Me; R3 = H, halogen, (C1-4)alkyl, CF3, or NO2; R4 = H, (C1-4)alkyl, halogen, OH, or NH2, with the proviso that R3 and R4 are not both H; and R5 = COOR5a wherein R5a = H or (C1-6)alkyl; or R5 is (C2-4)alkenylCOOR5a, (C1-4)alkylCOOR5a) or a salt or a prodrug, useful as inhibitors of HIV reverse transcriptase. For example, I (R = R1 = R4 = nul; R2 = Me, R3 = Et, R5 = CO2H) was prepared in a multistep process, starting from 2-chloro-3-nitropyridine and ethylamine to give 2-ethylamino-3-nitropyridine which was reduced and subsequently reacted with 5-bromo-2-chloro-3-pyridinecarbonyl chloride; the product was cyclized, reacted with allyltributylstannane, and then oxidized to II; II was reacted with Me 3-ethyl-4-hydroxybenzoate and saponified to give I (R = R1 = R4 = nul; R2 = Me, R3 = Et, R5 = CO2H) in 98 % yield.

Ι

RN 380378-91-6 HCAPLUS CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl-8-(2-propenyl)- (9CI) (CA INDEX NAME)

RN 380378-93-8 HCAPLUS
CN 3-Pyridinecarboxamide, 5-bromo-2-chloro-N-[6-chloro-2-(ethylamino)-3-pyridinyl]- (9CI) (CA INDEX NAME)

RN 380378-94-9 HCAPLUS
CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 2-chloro-11-ethyl-5,11-dihydro-5-methyl-8-(2-propenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{O} \\ & \text{N} & \text{N} & \text{CH}_2-\text{CH} = \text{CH}_2 \\ & \text{Cl} & \text{N} & \text{N} & \text{N} \end{array}$$

RN 380378-98-3 HCAPLUS

CN 2-Pyridinamine, N-ethyl-6-fluoro-3-nitro- (9CI) (CA INDEX NAME)

RN 380378-99-4 HCAPLUS

CN 2,3-Pyridinediamine, N2-ethyl-6-fluoro- (9CI) (CA INDEX NAME)

RN 380379-00-0 HCAPLUS

CN 3-Pyridinecarboxamide, 5-bromo-2-chloro-N-[2-(ethylamino)-6-fluoro-3-pyridinyl]- (9CI) (CA INDEX NAME)

RN 380379-01-1 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 8-bromo-11-ethyl-2-fluoro-5,11-dihydro-(9CI) (CA INDEX NAME)

RN 380379-02-2 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-2-fluoro-5,11-dihydro-5-methyl-8-(2-propenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \text{N} & \text{CH}_2 - \text{CH} = \text{CH}_2 \\ \\ \text{Et} & \text{Et} \end{array}$$

RN 380379-03-3 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-2-fluoro-5,11-dihydro-8-(2-hydroxyethyl)-5-methyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:117825 HCAPLUS

DOCUMENT NUMBER: 138:170259

TITLE: Preparation of dipyridodiazepinones as reverse

transcriptase inhibitors

INVENTOR(S):
Ogilvie, William W.; Deziel, Robert; O'Meara, Jeffrey;

Simoneau, Bruno

PATENT ASSIGNEE(S): Boehringer Ingelheim (Canada) Ltd., Can.

SOURCE: PCT Int. Appl., 71 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

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WO 2003011862
                                             WO 2002-CA1161
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
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             PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
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     EP 1414820
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                                             EP 2002-750729
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PRIORITY APPLN. INFO.:
                                             US 2001-308710P
                                                                 Р
                                                                    20010730
                                             WO 2002-CA1161
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                                                                    20020726
OTHER SOURCE(S):
                         MARPAT 138:170259
GI
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$$\mathbb{R}^{4} \mathbb{N}^{5} \mathbb{O}$$

$$\mathbb{N}^{1} \mathbb{N}$$

$$\mathbb{N}^{1} \mathbb{N}$$

$$\mathbb{N}^{1} \mathbb{N}$$

Title compds. [I; R2 = H, halo, NHNH2, alkyl, alkoxy, haloalkyl; R4 = H, Me; R5 = H, alkyl; R11 = alkyl, alkylcycloalkyl, cycloalkyl; Q = (substituted) naphthyl, fused phenylcycloalkyl, fused phenylheterocyclyl having 1-2 O, N, S], were prepared Thus, diisopropyl azodicarboxylate in THF was added dropwise to a mixture of 5,11-dihydro-11-ethyl-2-fluoro-5-methyl-8-(2-hydroxyethyl)-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, Ph3P, and 4-formyl-1-naphthol followed by stirring for 1 h to give 56% formylnaphthyl ether derivative, which was stirred with AgNO3 and NaOH in EtOH/THF to give 62% title compound I (Q = 4-carboxynaphthyl-1-yl; R2 = F; R4 = H; R5 = Me; R11 = Et) (II). II showed IC50<100 nM against wild type HIV-1 reverse transcriptase.

Ι

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of dipyridodiazepinones as reverse transcriptase inhibitors) 380379-03-3 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-2-fluoro-5,11-dihydro-8-(2-hydroxyethyl)-5-methyl- (9CI) (CA INDEX NAME)

RN

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:923799 HCAPLUS

DOCUMENT NUMBER: 136:37632

TITLE: Preparation of non-nucleoside reverse transcriptase

inhibitors

INVENTOR(S):
Simoneau, Bruno

PATENT ASSIGNEE(S): Boehringer Ingelheim (Canada) Ltd., Can.

SOURCE: PCT Int. Appl., 76 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	TENT	NO.			KIN	D	DATE			APPI	LICAT	ION :	NO.		D	ATE	
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WO	2001	0963	38		A1		2001	1220		WO 2	2001-	CA89	0		2	0010	614
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	RW:										, TZ,						
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BR	2001	0023	77		Α		2002	0219		BR 2	2001-	2377			2	0010	612 612 <
US	2002	0288	07		A1		2002	0307		US 2	2001-	8794	47		2	0010	612 <
US	6420	359			B2		2002	0716									
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EP	1294	720			A1		2003	0326		EP 2	2001 -	9491	2.4		21	2010	614
EP	1294	720			R1		2006	0405		•	, o o , i				_	0010	011
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			07		AZ		2003	0020		HU A	2003-	1102			21	3010	614
72	2004	5027	8 /		1		2004	0129		JP 2	2002-	5104	80		20	0010	614
EE	2002	0069	0		Α		2004	0615		EE 2	2002-	690			20	0010	614
NZ	5235	49			Α		2004	0827		NZ 2	2001- 2001-	5235	49		20	0010	614
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7.A	2002	0098	07		Δ		2003	1016		7A 1	2002-	9807	ے د		20	1021	202
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NO	2002	10 1150	1.1		Λ.		2004	1205	,	NO C	2001- 2001- 2002- 2002- 2002- 2002-	IU/3	30		21	JUZI.	203
MO	2002	0058	**		A		Z U U Z .	1205		NO 2	2002-	5844			20	0021	205

Roy P. Issac

HK 1057558 A1 20050408 HK 2004-100468 20040121 PRIORITY APPLN. INFO.: US 2000-212329P р 20000616 US 2000-256638P P 20001218 EP 2001-949124 A3 20010614 20010614 WO 2001-CA890

OTHER SOURCE(S): MARPAT 136:37632

GI

AB Compds. of formula I [R2 = H, F, Cl, (C1-4) alkyl, (C3-4) cycloalkyl, CF3; R4 = H, Me; R5 = H, Me, Et; R4 and R5 are not both Me, and if R4 is Me then R5 cannot be Et; R11 = Et, cyclopropyl, Pr, iso-Pr, isobutyl; Q = 4-or 5-quinolinyl or their 1-oxides] are prepared as inhibitors of HIV reverse transcriptase, wild-type and several mutant strains. Thus, II was prepared in several steps from 2-chloro-3-nitropyridine, ethylamine, 5-bromo-2-chloro-3-pyridinecarbonyl chloride and 4-hydroxyquinoline. II was shown to inhibit wild-type and mutant strains of reverse transcriptase in assays.

IT 330378-81-4P 380378-97-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dipyridodiazepinone derivs. as reverse transcriptase inhibitors)

RN 380378-81-4 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl-8-[2-[(1-oxido-4-quinolinyl)oxy]ethyl]- (9CI) (CA INDEX NAME)

RN 380378-97-2 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 2-chloro-11-ethyl-5,11-dihydro-5-methyl-8-[2-(4-quinolinyloxy)ethyl]-, mono(trifluoroacetate)

(9CI) (CA INDEX NAME)

CM 1

CRN 380378-63-2 CMF C25 H22 Cl N5 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

IT 390378-90-5P 380378-91-6P 380378-92-7P 380378-93-8P 380378-94-9P 380378-95-0P 380378-96-1P 380378-98-3P 380378-99-4P 380379-00-0P 380379-01-1P 380379-02-2P 380379-03-3P 380379-04-4P 380379-05-5P 380379-06-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of dipyridodiazepinone derivs. as reverse transcriptase inhibitors) 380378-90-5 HCAPLUS RN CN 3-Pyridinecarboxamide, 5-bromo-2-chloro-N-[2-(ethylamino)-3-pyridinyl]-(9CI) (CA INDEX NAME)

RN 380378-91-6 HCAPLUS
CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5methyl-8-(2-propenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
\text{Me} & \text{O} \\
\text{N} & \text{CH}_2 - \text{CH} = \text{CH}_2
\end{array}$$

RN 380378-92-7 HCAPLUS CN 2,3-Pyridinediamine, 6-chloro-N2-ethyl- (9CI) (CA INDEX NAME)

RN 380378-93-8 HCAPLUS
CN 3-Pyridinecarboxamide, 5-bromo-2-chloro-N-[6-chloro-2-(ethylamino)-3-pyridinyl]- (9CI) (CA INDEX NAME)

10/736,301>19/04/2007

RN 380378-94-9 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 2-chloro-11-ethyl-5,11-dihydro-5-methyl-8-(2-propenyl)- (9CI) (CA INDEX NAME)

RN 380378-95-0 HCAPLUS

CN 2-Pyridinamine, 6-chloro-N-cyclopropyl-3-nitro- (9CI) (CA INDEX NAME)

RN 380378-96-1 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 2-chloro-11-cyclopropyl-5,11-dihydro-8-(2-hydroxyethyl)-5-methyl- (9CI) (CA INDEX NAME)

RN 380378-98-3 HCAPLUS

CN 2-Pyridinamine, N-ethyl-6-fluoro-3-nitro- (9CI) (CA INDEX NAME)

380378-99-4 HCAPLUS RN

CN 2,3-Pyridinediamine, N2-ethyl-6-fluoro- (9CI) (CA INDEX NAME)

RN 380379-00-0 HCAPLUS

CN 3-Pyridinecarboxamide, 5-bromo-2-chloro-N-[2-(ethylamino)-6-fluoro-3-

pyridinyl] - (9CI) (CA INDEX NAME)

380379-01-1 HCAPLUS RN

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 8-bromo-11-ethyl-2-fluoro-5,11-dihydro- (9CI) (CA INDEX NAME) CN

RN380379-02-2 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-2-fluoro-5,11-

dihydro-5-methyl-8-(2-propenyl)- (9CI) (CA INDEX NAME)

10/736,301>19/04/2007

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \hline & \text{N} & \text{CH}_2 - \text{CH} = \text{CH}_2 \\ \hline & \text{Et} & \\ \end{array}$$

RN 380379-03-3 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-2-fluoro-5,11-dihydro-8-(2-hydroxyethyl)-5-methyl- (9CI) (CA INDEX NAME)

RN 380379-04-4 HCAPLUS

CN 3-Pyridinecarboxamide, N-(2,6-dichloro-4-methyl-3-pyridinyl)-2-(ethylamino)- (9CI) (CA INDEX NAME)

RN 380379-05-5 HCAPLUS

CN 3-Pyridinecarboxamide, 5-bromo-N-(2,6-dichloro-4-methyl-3-pyridinyl)-2-(ethylamino)- (9CI) (CA INDEX NAME)

RN 380379-06-6 HCAPLUS

CN 6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 8-bromo-2-chloro-11-ethyl-5,11-dihydro-4-methyl- (9CI) (CA INDEX NAME)

Roy P. Issac

10/736,301>19/04/2007

Roy P. Issac

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	45	"6037157"	US-PGPUB; USPAT	NEAR	ON	2007/04/19 18:13
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S1	1	((MICHAEL) near2 (CORDINGLEY)). INV.	US-PGPUB; USPAT	NEAR	ON	2007/04/19 18:12